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There is strong Air Force interest in compact, airborne, high-power generators and klystron/gyrotron/magnetron magnets. Both applications need superconducting magnets that can operate off robust cryocoolers at temperatures near liquid nitrogen (77K). The decisive element for all such applications is the conductor from which such magnets can be made. The material of choice is  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ , made in the form of a multilayer tape as a Coated Conductor (CC). Such conductors are multilayers of  $\sim 50 \mu\text{m}$ -thick Ni-alloy to support an  $\sim 1 \mu\text{m}$ -thick buffer layer (for now generally  $\text{Y}_2\text{O}_3/\text{YSZ}/\text{CeO}_2$ )  $\sim 2$ - $5 \mu\text{m}$   $\text{YBa}_2\text{Cu}_3\text{O}_x$  layer, all topped by a high-conductivity, normal-metal overlayer for stabilization and protection. The single most important characteristic of any CC is the need for texture in the superconductor so that blockage of current at grain boundaries is minimized. Texture is vital, since even low angle grain boundaries partially obstruct the current, reducing the global  $J_c$  and providing significant local sources of dissipation that may induce instabilities during magnet use. Understanding why grain boundaries block current and searching for ways to mitigate the problem forms the central thrust of this work.

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## Electromagnetic and Nanostructural Studies of Rare Earth Copper Oxide Grain Boundaries in High Temperature Superconductors

AFOSR Grant F49620-03-1

Final Report

November 1 2003 – October 31, 2006

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### OBJECTIVES

Our overall goal is to understand what controls the critical current density of low angle grain boundaries and to develop means to effectively ameliorate them, first in artificial bicrystal geometries and then in more realistic coated conductor geometries.

### Highlights

1. Our recent results on the effect of Ca-doping on the YBCO grain boundary atomic structure, chemistry and electromagnetic properties, were summarized in the paper **“Electromagnetic, atomic structure and chemistry changes induced by Ca-doping of low-angle  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  grain boundaries”**, *Nature Materials*, 4, 470-475 (2005). This article was highlighted in the *News and Views* section by the editor of Nature Materials and by the leading experts, Jochen Mannhart, from the University of Augsburg, Germany and by David Muller, from Cornell University whose comment *“Superconductors-Catching dopants in action”* emphasized the significance of our work for addressing the atomic mechanisms behind the beneficial effects of Ca doping on critical currents of YBCO grain boundaries. This New and Views article was highlighted on the cover page of the June 2005 issue of *Nature Materials*.
2. An important part of our Nature Materials paper was a new model of Ca segregation in the strain and electric field around low-angle grain boundaries. Our model predicts that the Ca distribution is highly inhomogeneous both along and across the boundary. We showed that the totality of our HREM TEM and EELS observations can be explained very well by quenched Cottrell atmospheres of solute Ca atoms segregated to the tensile regions at the dislocation cores. This segregation strongly reduces the local hole deficiency. In particular, this model explains our surprising result that, despite the significant expansion of the disordered region around the dislocation core, the critical current density of Ca doped  $5^\circ$  bicrystal is actually increased so much that the boundary becomes indistinguishable from the bulk, as far as the current transport is concerned. The model also explains the highly non-monotonic Ca profile across GB and predicts Ca-free current channels with no  $T_c$  suppression characteristic of Ca doped YBCO.

3. A complementary work, led by Xueyan Song, on faceting of low angle grain boundaries and atomic structure of the less-common [110] dislocation as well as atomic-scale structural changes induced by Ca-doping was accepted for *Journal of Materials Research* and will appear in 2007.
4. The next phase of our work is being undertaken by our graduate student Sang-Il Kim. He is in process of rebuilding our PLD system with a new chamber that will permit multi-target operation so that further alloying studies of grain boundaries can be pursued. We are particularly interested in studying the segregation of marginally doped alloying elements to grain boundaries, as noted in the case of Ca in paragraph 2 above. We started with variable Ca content and have found that the beneficial effects of Ca occur for 7-9° misorientations at smaller Ca contents of only 10%, as opposed to the optimum of 30% found to be optimum in the first experiments of Mannhart *et al.* at Augsburg on high angle grain boundaries (24-36°). This has served both to validate the charge and strain segregation model described in paragraph 2 above and to show that the beneficial effects of can be obtained with a smaller degree of  $T_c$  depression that occurs with 30% substitution for Y.
5. The segregation model was then used to design a series of RE-alloyed grain boundaries using the size of the RE ion as the variable. We are particularly interested in the use of small and large RE ions such as Yb (small) and Nd (large). We predict beneficial effects from Yb and will test this out early in 2007 after we have moved the PLD system to Florida State University.
6. An extensive array of coated conductors studies, including some individual grain boundary studies performed by isolating individual grain boundaries within coated conductors have been performed by Matt Feldmann, partly using the resources of this award but predominantly under MURI support.

#### Publications:

1. S.I. Kim, D.M. Feldmann, D.T. Verebelyi, W. Zhang, X. Li, C. Thieme, A.A. Polyanskii, and D.C. Larbalestier, "Influence of the grain boundary network on the critical current density of deformation-textured MOD YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> coated conductors," *Physical Review B* **71**, 104501-1-9. (2005.)
2. X. Song, G. Daniels, D.M. Feldmann, A. Gurevich, and D.C. Larbalestier, "Electromagnetic, Atomic-Structure and Chemistry Changes Induced by Ca-doping of Low Angle YBCO Grain Boundaries," *Nature Materials*, **4**, 470-475. (2005).
3. D.M. Feldmann, D.C. Larbalestier, T. Holesinger, R. Feenstra, A.A. Gapud, E.D. Specht. "Evidence for extensive grain boundary meander and overgrowth of substrate grain boundaries in high critical current density ex situ YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> coated conductors." *J. Mater. Res.*, **20**, 2012-2020. (2005.)
4. D.M. Feldmann, T.G. Holesinger, C. Cantoni, R. Feenstra, N.A. Nelson, D.C. Larbalestier, D.T. Verebelyi, X. Li X, M. Rupich. "Grain orientations and grain boundary networks of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> films deposited by metalorganic and pulsed laser deposition on biaxially textured Ni-W substrates." *J. Mater. Res.* **21**, 923 (2006).
5. X. Song, "(110) Facets and dislocation structure of low-angle grain boundaries in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> and Y<sub>0.7</sub>Ca<sub>0.3</sub>Ba<sub>2</sub>Cu<sub>3</sub>O<sub>7-d</sub> thin film bicrystals." To appear in *Journal of Materials Research*, **22**, xxxx (2007).